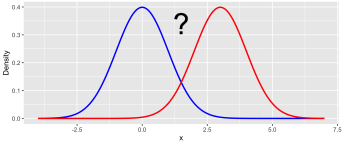
Introduction to Machine Learning

KL for ML

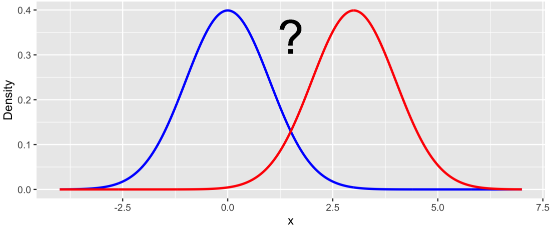


Learning goals

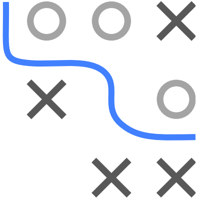
- Understand why measuring distribution similarity is important in ML
- Understand the advantages of forward and reverse KL

MEASURING DISTRIBUTION SIMILARITY IN ML

- Information theory provides tools (e.g., divergence measures) to quantify the similarity between probability distributions

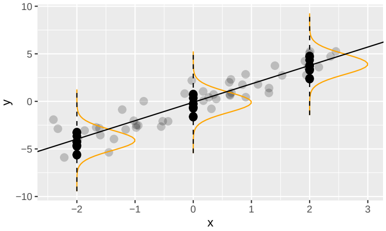


- The most prominent divergence measure is the KL divergence
- In ML, measuring (and maximizing) the similarity between probability distributions is a ubiquitous concept, which will be shown in the following.



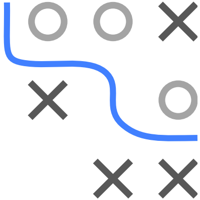
MEASURING DISTRIBUTION SIMILARITY IN ML

- **Probabilistic model fitting**
  Assume our learner is probabilistic, i.e., we model $p(y|\mathbf{x})$ (for example, logistic regression, Gaussian process, ...).

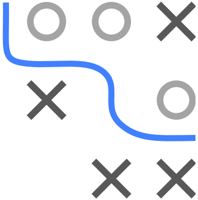


We want to minimize the difference between $p(y|\mathbf{x})$ and the conditional data generating process $\mathbb{P}_{y|\mathbf{x}}$ based on the data stemming from $\mathbb{P}_{y,\mathbf{x}}$.

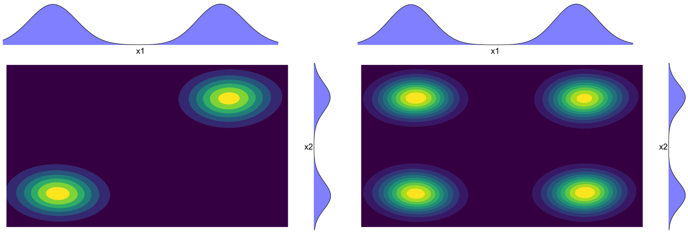
Many losses can be derived this way. (e.g., cross-entropy loss)



MEASURING DISTRIBUTION SIMILARITY IN ML



- **Feature selection** In feature selection, we want to choose features the target strongly depends on.



We can measure dependency by measuring the similarity between $p(\mathbf{x}, y)$ and $p(\mathbf{x}) \cdot p(y)$.

We will later see that measuring this similarity with KL leads to the concept of mutual information.

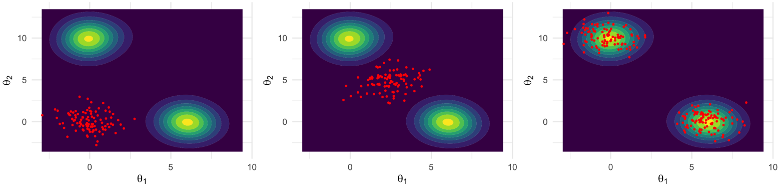
MEASURING DISTRIBUTION SIMILARITY IN ML

- **Variational inference (VI)** By Bayes' theorem it holds that the posterior density

$$p(\theta|\mathbf{X}, \mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{X}, \theta)p(\theta)}{\int p(\mathbf{y}|\mathbf{X}, \theta)p(\theta)d\theta}.$$

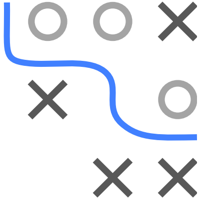
However, computing the normaliziation constant $c = \int p(\mathbf{y}|\mathbf{X}, \theta)p(\theta)d\theta$ analytically is usually intractable.

Sampling from q(x)



In VI, we want to fit a density q_ϕ with parameters ϕ to $p(\theta|\mathbf{X}, \mathbf{y})$.

KL DIVERGENCE



Divergences can be used to measure the similarity of distributions.

For distributions p, q they are defined such that

1. $D(p, q) \geq 0$,
2. $D(p, q) = 0$ iff $p = q$.

$\Rightarrow$ divergences can be (and often are) non-symmetrical.

If the same measure dominates the distributions p, q, we can use KL.
For a target distribution p and parametrized distribution q_ϕ, we call

- $D_{KL}(p \| q_\phi)$ forward KL,
- $D_{KL}(q_\phi \| p)$ reverse KL.

In the following, we highlight some properties of the KL that make it attractive from an ML perspective.

KL DIVERGENCE

- **Forward KL for probabilistic model fitting**
  We have samples from the DGP $p(y, \mathbf{x})$ when we fit our ML model.

  If we have a probabilistic ML model q_ϕ the expected forward KL

$$\mathbb{E}_{\mathbf{x}\sim p_\mathbf{x}} D_{KL}(p(\cdot|\mathbf{x})||q_\phi(\cdot|\mathbf{x})) = \mathbb{E}_{\mathbf{x}\sim p_\mathbf{x}} \mathbb{E}_{y\sim p_{y|\mathbf{x}}} \log\left(\frac{p(y|\mathbf{x})}{q_\phi(y|\mathbf{x})}\right).$$

  We can directly minimize this objective since

$$\begin{aligned}\nabla_\phi \mathbb{E}_{\mathbf{x}\sim p_\mathbf{x}} D_{KL}(p(\cdot|\mathbf{x})||q_\phi(\cdot|\mathbf{x})) &= \mathbb{E}_{\mathbf{x}\sim p_\mathbf{x}} \mathbb{E}_{y\sim p_{y|\mathbf{x}}} \nabla_\phi \log\left(p(y|\mathbf{x})\right) \\ &\quad - \mathbb{E}_{\mathbf{x}\sim p_\mathbf{x}} \mathbb{E}_{y\sim p_{y|\mathbf{x}}} \nabla_\phi \log\left(q_\phi(y|\mathbf{x})\right) \\ &= -\nabla_\phi \mathbb{E}_{\mathbf{x}\sim p_\mathbf{x}} \mathbb{E}_{y\sim p_{y|\mathbf{x}}} \log\left(q_\phi(y|\mathbf{x})\right)\end{aligned}$$

  $\Rightarrow$ We can estimate the gradient of the expected forward KL without bias, although we can not evaluate $p(y|\mathbf{x})$ in general.

KL DIVERGENCE

- **Reverse KL for VI**
  Here, we know our target density $p(\boldsymbol{\theta}|\mathbf{X}, \mathbf{y})$ only up to the normalization constant, and we do not have samples from it.

  We can directly apply the reverse KL since for any $c \in \mathbb{R}_+$

$$
\begin{aligned}
\nabla_\phi D_{KL}(q_\phi \| p) &= \nabla_\phi \mathbb{E}_{\boldsymbol{\theta} \sim q_\phi} \log \left(\frac{q_\phi(\boldsymbol{\theta})}{p(\boldsymbol{\theta})} \right) \\
&= \nabla_\phi \mathbb{E}_{\boldsymbol{\theta} \sim q_\phi} \log \left(\frac{q_\phi(\boldsymbol{\theta})}{p(\boldsymbol{\theta})} \right) - \underbrace{\nabla_\phi \mathbb{E}_{\boldsymbol{\theta} \sim q_\phi} \log c}_{=0} \\
&= \nabla_\phi \mathbb{E}_{\boldsymbol{\theta} \sim q_\phi} \log \left(\frac{q_\phi(\boldsymbol{\theta})}{c \cdot p(\boldsymbol{\theta})} \right).
\end{aligned}
$$

  $\Rightarrow$ We can estimate the gradient of the reverse KL without bias (even if we only have an unnormalized target distribution)

KL DIVERGENCE

The asymmetry of the KL has the following implications

- Forward KL $D_{KL}(p \| q_\phi) = \mathbb{E}_{\mathbf{x} \sim p} \log \left(\frac{p(\mathbf{x})}{q_\phi(\mathbf{x})} \right)$ is mass-covering since $p(\mathbf{x}) \log \left(\frac{p(\mathbf{x})}{q_\phi(\mathbf{x})} \right) \approx 0$ if $p(\mathbf{x}) \approx 0$ and $q_\phi(\mathbf{x}) \not\gg p(\mathbf{x})$.
- Reverse KL $D_{KL}(q_\phi \| p) = \mathbb{E}_{\mathbf{x} \sim q_\phi} \log \left(\frac{q_\phi(\mathbf{x})}{p(\mathbf{x})} \right)$ is mode-seeking (zero-avoiding) since $q_\phi(\mathbf{x}) \log \left(\frac{q_\phi(\mathbf{x})}{p(\mathbf{x})} \right) \gg 0$ if $p(\mathbf{x}) \approx 0$ and $q_\phi(\mathbf{x}) > 0$

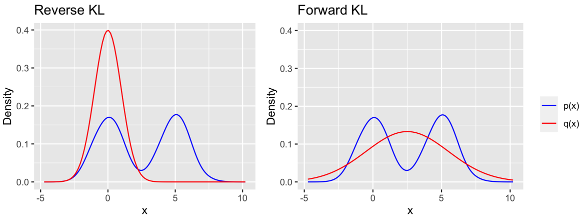


Figure: Optimal q_ϕ when q_ϕ is restricted to be Gaussian.